Supporting Information

Screening for DNA Adducts by Data-Dependent Constant Neutral Loss - Triple Stage (MS^3) Mass Spectrometry with a Linear Quadrupole Ion Trap Mass Spectrometer

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Supporting Information – Figure Captions

Figure S-1. Structures of genotoxicants under investigation.

Figure S-2. The 2nd-generation product ions of guanyl-4-ABP at *m/z* 277.1 $[BH_2 - 42]^+$ and *m/z* 249.1 $[BH_2 - 70]^+$ at MS^4 scan stage.

Figure S-3. The 2nd-generation product ions of the proposed guanyl-N^2-N^4-ABP ion at *m/z* 210.3 $[BH_2 - 109]^+$ at the MS^4 scan stage (see Scheme S-1).

Figure S-4. The 2nd-generation product ions of adenyl-4-ABP adduct at *m/z* 276.1 $[BH_2 - 27]^+$ at the MS^4 scan stage.

Figure S-5. Targeted CNL-MS^3 data-dependent scanning of 4-ABP adducts in human hepatocytes treated with 4-ABP (10 μM). The data-dependent CNL-MS^3 chromatograms for dA-ABP adducts (upper chromatogram) and dG-ABP adducts (lower chromatogram) are presented. The respective t_R and area of response of the ion counts are shown. Untreated hepatocytes showed no peaks at these transitions (data not shown).

Figure S-6. CNL-MS^3 data-dependent product ion spectra of isomeric dA-ABP adducts formed in human hepatocytes.

Scheme S-1. The proposed mechanism of several 2nd-generation product ions derived from the fragmentation of the *m/z* 210.3 ion $[BH_2 - 109]^+$ of the proposed guanyl-N^2-N^4-ABP adduct, at the MS^4 scan stage (see Figure S-3).